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Neutronic Analysis Needs for Future Nuclear Energy Systems

Presented at

Workshop on the Role of Simulation in Nuclear Energy
Livermore, CA
December 15, 2005

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THE UNIVERSITY OF CHICAGO
Office of Science
U.S. DEPARTMENT OF ENERGY

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Topics

- **Relevance of neutronic analysis to goals for future systems**
- **Observations on current status of neutronic analysis**
  - **Conventional approach and approximations**
  - **Typical accuracies**
- **Future nuclear energy system options**
  - **Physics distinctions and analysis issues**
- **Work underway in Generation IV program to meet analysis needs**
- **Experimental needs and relevant activities**

Neutronic Analysis is Key to Meeting Goals for Future Systems

Economics	• Compact core and shield configuration • Minimum fissile and reactivity control requirements • Fuel management optimization (e.g. cycle length)
Sustainability	• Achievement of high average burnup (resource utilization for once through cycle) • Waste characteristics (toxicity, decay heat)
Safety & Reliability	• Verifying fission power & decay heating within heat removal capabilities • Excess reactivity minimization, favorable reactivity Δ's for temperature and material density changes
Proliferation Resistance & Physical Protection	• Accurate accounting for life-cycle flows of fissile materials into and out of reactor • Isotopic makeup (weapons attractiveness)

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Neutronics Analysis: Overall Status

- **Theory and governing equations are well known**
- **Nuclear data are for the most part well known**
  - Sometimes “adjusted” within their uncertainty ranges
- **Geometry and composition have stochastic uncertainty and are affected by thermal, mechanical, irradiation, and chemical phenomena**
  - These other “coupled” phenomena are not as well described, but they can dominate the analysis errors
- **Neutronic analysis challenge is <u>efficient solution</u>, taking into account geometric complexity and energy dependence of nuclear data**
- **Monte Carlo method can represent these details, <u>but</u>**
  - Computer resource requirements remain unmanageable for many types of routine analyses (local reaction rates, effects of small perturbations, transients, …)
  - Need sufficiently low uncertainty, <u>reliable variance estimates and uncertainty propagation</u>

Neutronics Analysis: Overall Status, cont'd

- **Computer limitations have motivated development of clever approximations and sophisticated procedures**
  - They are tailored to specific systems and analyses
  - They work well within their applicability/validity ranges
  - High degree of user competence is essential

Conventional approximations

- **Detailed space-energy-direction analysis performed for a repeated portion of the geometric domain (lattice physics)**
  - With assumed/approximated boundary conditions
  - Space/energy condensed parameters defined and tabulated for global "homogenized" model
  - Global model analyzed in 3-D with low-order approximation of Boltzmann equation
    - *Goal is to match detailed solution, in integral sense*
  - Detailed information recovered by reconstruction (de-homogenization) methods
- **Nuclide depletion and buildup modeled using quasi-steady model**
  - Depletion steps are ~ days
- **Faster transients modeled with condensed (often single point) model for time-dependent amplitude**
  - Accuracy depends on frequency of kinetic-parameter and space-energy-direction flux shape recalculation

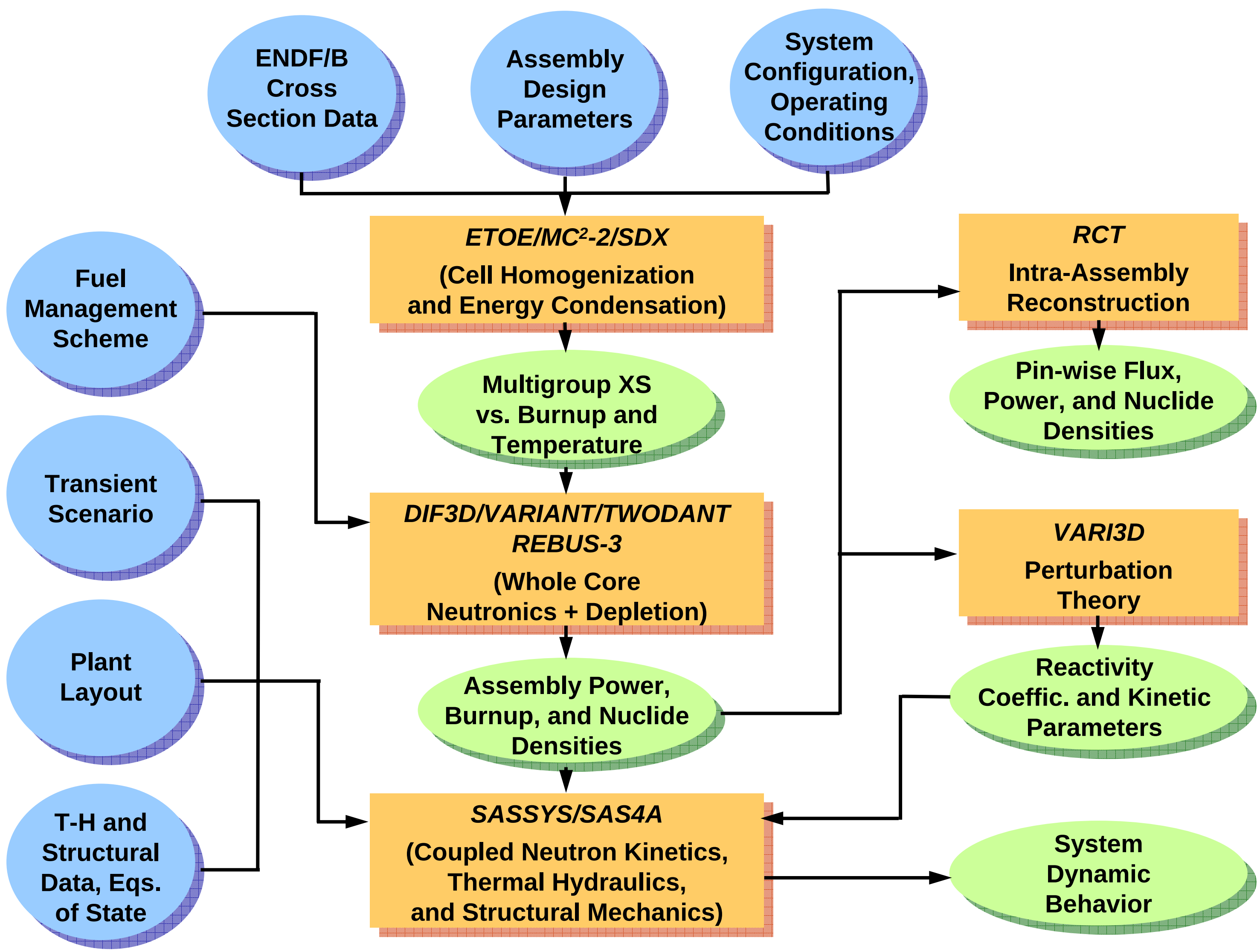
Uncertainty in Predictions

	Current	Future ?
Multiplication factor, k-eff	0.5%	<0.1%
Local power density	~5%	~1%
Control element worth	2-10%	1%
Reactivity coefficients:		
Large effects	10%	1-5%
Small effects	20%	10%
Kinetics parameters	5%	2%
Local nuclide densities:		
Major constituents	5%	1%
Minor constituents	10-20%	2-5%

Status of Neutronic Analysis Tools by Reactor Type

- **Among different reactor types, the neutronic methods, codes and databases for Light Water Reactors are by far the most advanced and thoroughly tested**
  - Extensively developed by commercial sector
  - On-line and off-line capabilities available, with coupling to T-H
  - Fast running models employed in optimization software
  - Extensively qualified, through hundreds of reactor-years of application experience
- **Fast reactor tools are somewhat less well developed and validated**
  - Concerted efforts at ANL through late 1980's
  - French CEA has in recent years advanced the state-of-art
- **Neutronic tools for gas-cooled reactors significantly lag in their development and validation status**
  - Until recently, in Generation IV program, little contemporary effort worldwide

Example: ANL Fast Reactor Code Suite



Candidate Future Systems (Gen IV)

System	Neutron Spectrum	Fuel Cycle	Size	Applications	R&D
Very High Temp. Gas Reactor (VHTR)	*Thermal*	*Open*	*Med*	*Electricity, Hydrogen Production, Process Heat*	*Fuels, Materials, H_2 production*
Supercritical Water Reactor (SCWR)	*Thermal, Fast*	*Open, Closed*	*Large*	*Electricity*	*Materials, Safety*
Gas-Cooled Fast Reactor (GFR)	*Fast*	*Closed*	*Med to Large*	*Electricity, Hydrogen, Actinide Management*	*Fuels, Materials, Safety*
Lead-alloy Cooled Fast Reactor (LFR)	*Fast*	*Closed*	*Small*	*Electricity, Hydrogen Production*	*Fuels, Materials compatibility*
Sodium Cooled Fast Reactor (SFR)	*Fast*	*Closed*	*Med to Large*	*Electricity, Actinide Management*	*Advanced Recycle*
Molten Salt Reactor (MSR)	*Thermal*	*Closed*	*Large*	*Electricity, Hydrogen, Actinide Management*	*Fuel, Fuel treatment, Materials, Safety and Reliability*

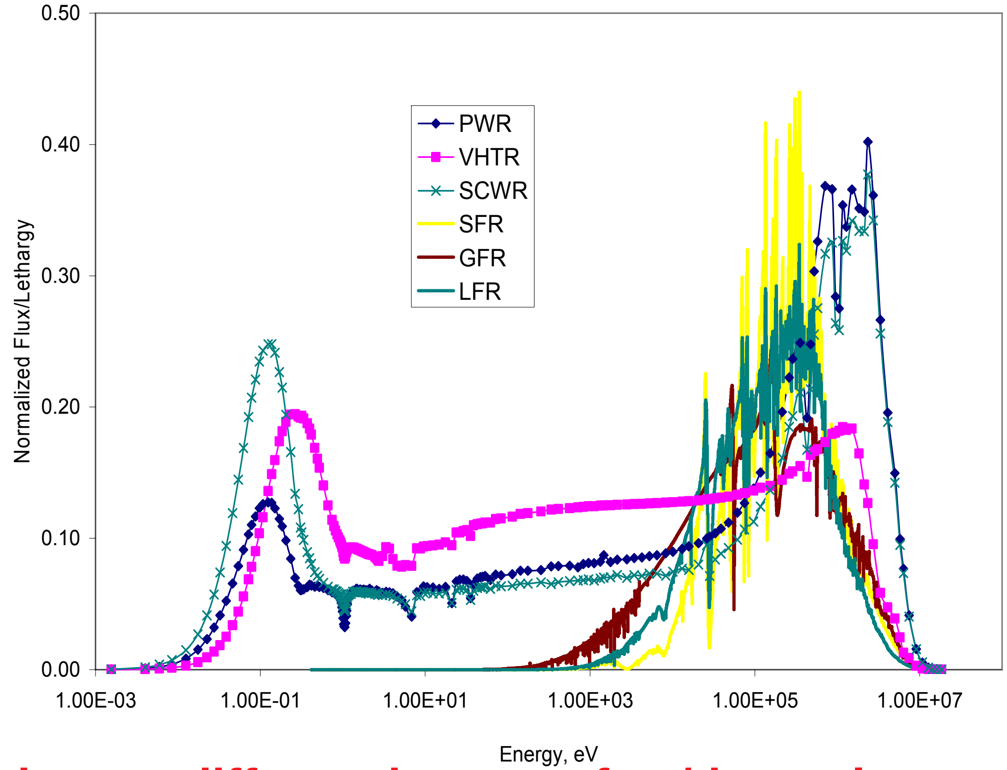
Note: Neutronics not a feasibility issue for any Gen IV system

Physics of Advanced Reactors - #1
Comparison of Neutron Energy Spectra

- **In short-term (decades), LWRs will be the dominant reactor type**
  - **Only existing reactor type – U.S. capacity of ~100 GWe**
  - **Early replacement plants will likely be advanced LWRs (ALWRs)**

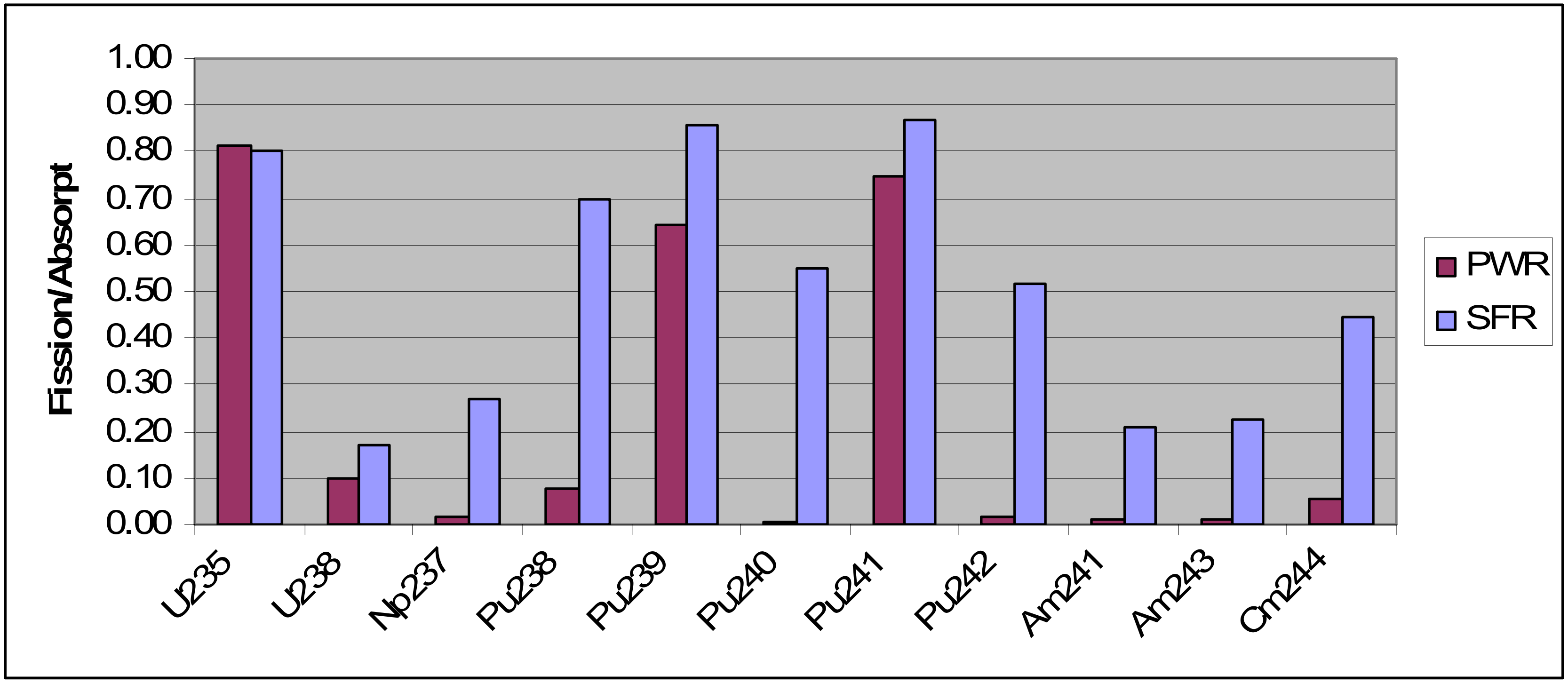
- **In LWRs, neutrons are moderated by water**
- **Fission reactions occur in the "thermal" peak**
- **Carbon moderated GCRs has more epithermal neutrons**

- **In fast reactors, moderators are eliminated**
- **Fission reactions occur in the "fast" energy range**



Actinide transmutation behavior is very different between fast/thermal

Physics of Advanced Reactors - #2
Fission-to-Absorption Ratio for PWR and SFR



- **Fissile isotopes are likely to fission in both thermal/fast spectrum**
  - **Fission fraction is higher in fast spectrum**
- **Significant (up to 50%) fission of fertile isotopes in fast spectrum**

Net result is more excess neutrons generated by fast fission

Physics of Fast Reactor Design - #3
Comparison of Key Cross Sections

Reaction	Thermal Concepts			Fast Concepts		
	PWR	**VHTR**	**SCWR**	**SFR**	**LFR**	**GFR**
U238c	0.91	**4.80**	0.95	0.20	0.26	0.32
Pu239f	89.2	164.5	138.8	1.65	1.69	1.90
P239f/U238c	**97.7**	34.3	146.6	**8.14**	**6.59**	**6.00**
Fe	0.4			0.007		
Fission Prod.	90			0.2		

- **In VHTR, large U-238 capture cross section from epithermal neutrons**
- **In fast spectrum, U-238 capture is more prominent (low P239f/U238c)**
  - **A much higher enrichment is required to achieve criticality**
- **The parisitic capture cross section of structure and fission products is much higher in a thermal spectrum**
  - **Internal and/or external conversion of U-238 is enhanced in FRs**
  - **FRs can use conventional structural materials (stainless steel)**

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Implications of Differences in Advanced Reactor Physics

- **Different missions result from the physics distinctions**
  - **Thermal reactors are typically configured for LEU utilization in <u>once-through (open) fuel cycle</u>**
  - **Fast reactors are typically intended for <u>closed fuel cycle</u> with uranium conversion and resource extension**
- **Different phenomena are important for each system:**
  - **Dominant energy range of neutron interactions**
  - **Relative importance of U-238 capture**
  - **Leakage fraction and reflector importance**
  - **Impact of fission product poisoning**
  - **Generation rate of higher actinides**

Thus, a key question is the approach to improved simulation with 2 options

1. **A univeral code to simulate the neutronics of all reactor types**
2. **Specific modules to simulate the key issues for a given system type**

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Summary of Physics Analysis Issues

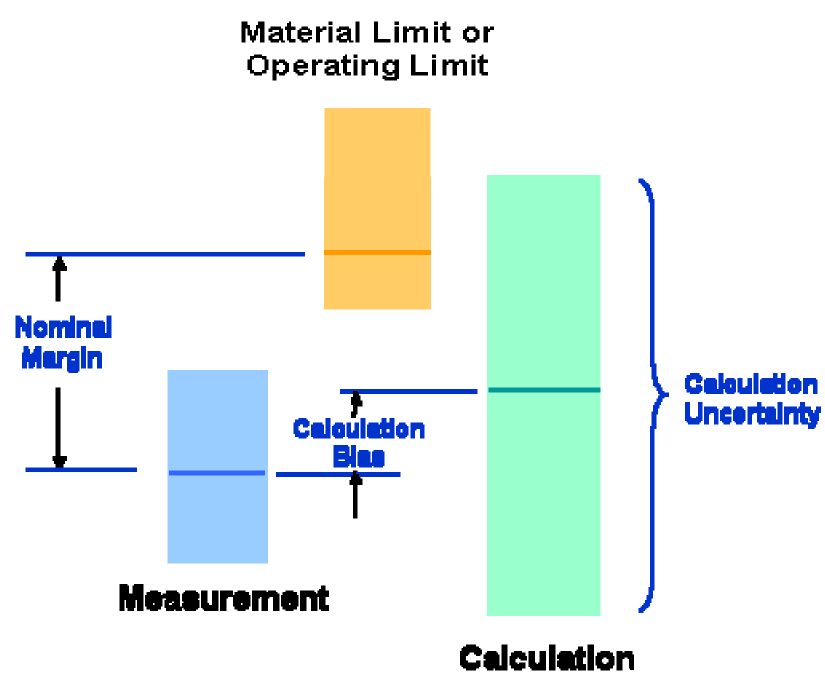
<table>
<tr><th>System</th><th colspan="2">Neutronic Analysis Issues</th></tr>
<tr><td>VHTR</td><td>• Fuel double heterogeneity
• Stochastic behavior of pebble movement (for PBR variant)</td><td>• Graphite scattering treatment
• Neutron streaming through coolant channels
• Core/reflector interfacial effect</td></tr>
<tr><td>GFR</td><td colspan="2" rowspan="3">• Data for actinides, coolant (e.g., Pb, Bi) and fuel matrix candidate materials
• Neutron streaming
• Full-core transport effects
• Spectral transition at core periphery
• Modeling of reactivity feedback coefficients including expansion feedback</td></tr>
<tr><td>LFR</td></tr>
<tr><td>SFR</td></tr>
<tr><td>SCWR</td><td>• Similar to BWRs
• Increased heterogeneity</td><td>• Strong coupling of neutronics and T-H
• Neutron streaming</td></tr>
<tr><td>MSR</td><td>• Evolution of mobile-fuel composition
• Delayed neutron precursor loss</td><td>• Modeling of nuclear, thermal, and physio-chemical processes</td></tr>
</table>

Rationale for Improving Physics Analysis Methods

- Enable accurate predictions of system performance
  - Define service conditions for fuels, materials, and components
  - Quantify performance advances relative to current generation systems
  - Increase assurance of performance gains, <u>prior to system operation</u>

- Reliably characterize and reduce modeling uncertainties, which necessitate over-conservatism in design
  - Avoid potentially costly efforts to improve upon the capabilities of available technologies

- Enhance prospects for regulatory acceptance of new system features



Rationale, cont'd

- **Once system is operating, some conditions can be measured and some can be controlled**
  - On line (e.g., power & flows)
  - At maintenance intervals (fuel loading)
- **Addition of measurement instruments and control degrees of freedom is expensive**
  - Off-line and on-line calculations still needed to determine, e.g., peak conditions of temperature, burnup, radiation damage, etc.
- **For off-normal conditions (accidents) and prior to system operation, <u>only</u> calculations are available**
  - Only means of providing a-priori assurance of performance

Approach Taken in DOE-NE Gen IV Program

- **Specify analytical capabilities needed to design Gen IV systems and characterize their performance**
  - Data
  - Models
  - Software/codes
  - Analysis procedures

- **Identify <u>relevant, high-quality</u> validation measurements**

- **Assess the adequacy of existing simulation tools <u>and</u> measurements**

- **Implement and qualify required improvements**
  - Building on existing capabilities
  - Budget-constrained, evolutionary approach

- **Three workshops on Gen IV analysis needs and capabilities were conducted in 2003:**
    - ***Reactor physics design analysis*** ***Feb 18-19, at ANL***
    - ***T-H and safety analysis*** ***Mar 18-19, at INEEL***
    - ***Nuclear data needs*** ***Apr 24-25, at BNL***
  - **Attended by lab, university and industry representatives**
  - **Conclusions and recommendations documented**
  - **Outcome factored into Generation IV program plan**

- **Subsequent workshops**
  - **International workshop on reactor physics, at PHYSOR Topical Meeting (April 2004, Chicago)**
  - **International workshop on nuclear data needs (April 2005, Antwerp)**
  - **Workshop on requirements and capabilities for CFD analysis of advanced, gas-cooled reactors, at ASME Fluids Engineering Summer Conference (June 22, 2005, Houston)**

- **Significant incentive identified to improve upon the older tools currently available for analysis of gas cooled reactors**
  - **Increase modeling fidelity, efficiency and user friendliness**
  - **Verify and validate predictions to modern standards**

Examples of Physics Modeling Needs Identified in Workshops

- **Representation of double heterogeneity of coated particle fuels**
- **Simulation of systems with moving fuel (<u>PBRs</u>, MSRs)**
- **Accurate modeling of spectral transition regions at core/reflector interface**
- **Analysis of small cores with significant global transport effects**
- **Reliable estimation of reactivity feedback from expansion or displacement of reactor components**
- **Validation of nuclear data for minor actinides, non-standard reactor materials**
- **Reliable estimation of materials damage parameters for in-core and ex-core structures**
- **Accurate resolution of detailed SS and transient power, flow, and temperature distributions (reduce hot channel factors)**

Experimental Needs in Neutronics: Differential Nuclear Data

- **Transuranic actinide nuclides**
- **Non-conventional coolant, structure and fuel matrix materials employed by LFR and GFR concepts**
  - Examples: Pb, Bi, Si, Mo, Nb
- **Sensitivity analysis used to identify the key isotopes, energy ranges, and impact on accuracy**

Experimental Needs in Neutronics: Integral Data

- **Available from measurements at experimental facilities, test reactors, and operating (power) reactors**
  - Provide combined test of data, methods, and software implementation
- **Key generic needs**
  - Accurate measurement, small and well characterized uncertainty
  - Relevance/similarity to design configuration of interest
  - Sensitivity to important parameters (that are uncertain)
- **Measurements are planned at CEA-Cadarache (MASURCA facility) to validate neutronic predictions for gas-cooled fast reactors (GFR)**
  - ENIGMA program
- **Need to examine large historical database to identify gaps and future needs**
  - Critical experiment facilities allow high precision-measurements but typically don't allow simulation of thermal or irradiation effects
  - Operating reactors: measurement often too intrusive and imprecise
- **Anticipate greatest payoff from well targeted integral measurements**
  - e.g., reactivity worth of a particular nuclide in a well characterized energy spectrum)

Summary

- **Neutronics of nuclear systems can be modeled quite well**
  - For most limiting desing parameters, non-neutronic phenomena and error sources dominate
- **Physics issues are different between the reactor options**
  - Universal tool would need to be comprehensive
  - Tailored simulation modules may be a preferable approach
- **Improvement of neutronics is motivated mainly by need to better characterize and improve performance**
  - Within operating limits of fuels, materials, and components
- **Some efforts are underway to improve neutronic analysis capabilities for future systems in the DOE Generation IV program**
  - Evolutionary approach, building on existing capabilities
  - Significant emphasis on high-quality measurements needed to verify improvements

Extras

Reactor Characteristics

	VHTR	SCWR	GFR	LFR	SFR
Power, MW_{th}	600-800 (block) ~300 (pebble)	~2000-3800	600, 2400	25-400	600-3500
Power Density, W/cm^3	≤ 6.5	≤ 70	100 (50-200)	25-100	200-400
Primary Coolant (T_{Outlet}, °C)	He (1000) Molten Salt?	SC H_2O (430-500)	He (800-850) SC CO_2	Pb (500-800) Pb-Bi (500-550)	Na (510-550)
Fuel Material	UO_2, $UC_{0.5}O_{1.5}$	UO_2	(U,TRU) carbide, nitride, oxide	(U,TRU) nitride	(U,TRU) oxide, metal alloy
Fuel Form	Triso particle	solid pellet	CerCer dispersion, solid solution, coated particle	solid pellet	pellet or slug
Fuel Element/ Assembly	hex block, pebble	LWR or AGR type pin bundle	hex block, plate, pin, or particle	triangular pitch pin bundle	triangular pitch pin bundle w/duct
Moderator	graphite	water rods (PV) D_2O (PT)	None	None	None
Core Structural Material	graphite	F-M SS, Ni alloy	SiC matrix or cladding, TiN, ODS steel	F-M SS, SiC/SiC composite	ODS ferritic steel

Suggested Priorities for Future Work: Nuclear Data

(From Gen IV Workshops)

- Systematically assess needs for further evaluation and measurement
  - Pu, MA, Pb, Bi, unconventional GFR fuel matrix and reflector materials
  - Consider contributions of different materials/reactions to the uncertainty in key performance parameters
  - Requires covariance data in format suitable for application studies
- Compare high fidelity calculations (deterministic and Monte Carlo) to integral measurements sensitive to materials/reactions in question
  - Provides validation data in integral sense
  - Ensemble of measurements indicates adjustments to data and their correlated uncertainties

Priority should be placed on identifying past integral experiment measurements of greatest relevance to future systems and on preserving their specifications and measured results

Additional experiments to address identified discrepancies

Suggested Priorities for Future Work: Modeling Capabilities

- For gas-cooled reactors, test and improve capabilities for physics analysis and design optimization
  - Treatment of the double heterogeneity and random distribution of particles
  - Accounting for the stochastic nature of pebble flow (for the PBR variant)
  - Mutually consistent flux and thermal-fluidic conditions

- For fast reactors, assess and implement modeling procedures that accurately represent
  - Spectral transitions at core periphery
  - Neutron streaming in low-coolant density configurations
  - Reactivity effects of thermal or radiation induced displacement of core structures

- Implement and qualify standardized methods for computing dpa and for correlating damage (macroscopic manifestation) to dpa

Suggested Priorities for Future Work: Modeling Capabilities (cont'd)

- **Advance Monte Carlo simulation capabilities**
  - **Improve reliability of variance estimates**
  - **Estimate and propagate nuclide density uncertainties in depletion calculations**
  - **Speed up simulation, e.g., through improved variance reduction techniques and effective use of increasing computer capabilities**

- **Improve efficiency (foremost human, but also machine effort)**
  - **Greater automation, modularization, standardization of interfaces**
  - **Example: interpolation of nuclear data to specified temperature in MC simulation**